Thermodynamics of Spin-1/2 Heisenberg Chains: Experiment and Theory

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Collaborators

Experiment

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Theory

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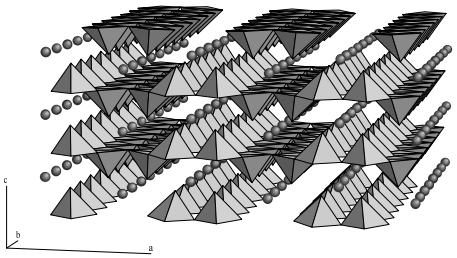
Introduction

We have measured the magnetic susceptibility χ and/or specific heat $C_p(T)$ of two insulating compounds containing spin S = 1/2 chains: NaV_2O_5, and the ambient- (AP) and high-pressure (HP) forms of $(VO)_2P_2O_7$

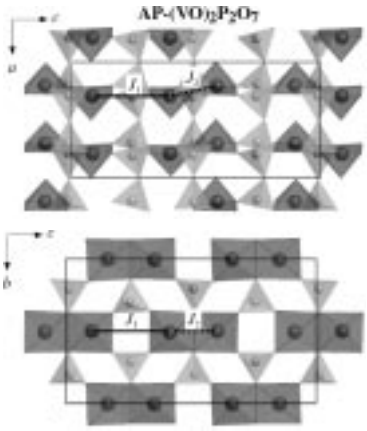
NaV_2O_5 is structurally a two-leg spin ladder compound with one electron per V-O-V rung. According to theory, the ladder can be mapped onto a spin-1/2 chain problem. NaV_2O_5 undergoes combined charge, lattice, and spin dimerization transitions at T_c = 34 K.
Goals: (1) Measure $\chi(T)$ and $C_p(T)$ on good single crystals of NaV_2O_5. (2) Compute the temperature-dependent spin gap Δ below T_c from the $\chi(T)$ data and compare the results with those of other measurements such as neutron scattering. (3) From the $C_p(T)$ data, determine the relative contributions of the spin and charge/lattice degrees of freedom to the phase transition at T_c

Structure of NaV_2O_5



$(VO)_2P_2O_7$: DCJ discovered in **1987** that this S = 1/2 compound has a spin gap, and fitted his $\chi(T)$ data by existing theoretical predictions for $\chi(T)$ of the spin-1/2 AF alternating-exchange chain. The crystal structure suggests that the compound contains two-leg V spin ladders instead, but no predictions for $\chi(T)$ of spin ladders existed at that time
1994: Barnes and Riera fitted DCJ's $\chi(T)$ data by a two-leg ladder model. Inelastic neutron scattering measurements on a powder by Eccleston et al. confirmed the spin ladder model
1997: Garrett et al. ruled out the spin ladder model and re-confirmed the alternating chain model from inelastic neutron scattering data on single crystals. A "troublesome" second spin gap was found, not possible for the alternating chain model, which was attributed to two-magnon bound states
1999: Yamauchi et al. deduced from NMR that $(VO)_2P_2O_7$ contains two independent alternating-exchange chains, with the two spin gaps as found in the neutron measurements on single crystals
1999: Azuma et al. discovered a high-pressure phase of $(VO)_2P_2O_7$ with a simpler structure containing a single type of alternating-exchange chain
Goals: (1) Measure the $\chi(T)$ of powders and single crystals of the ambient- (AP) and high-pressure (HP) phases of $(VO)_2P_2O_7$ and (2) test consistency with the two- and one-chain models, respectively

Structure of AP-$(VO)_2P_2O_7$

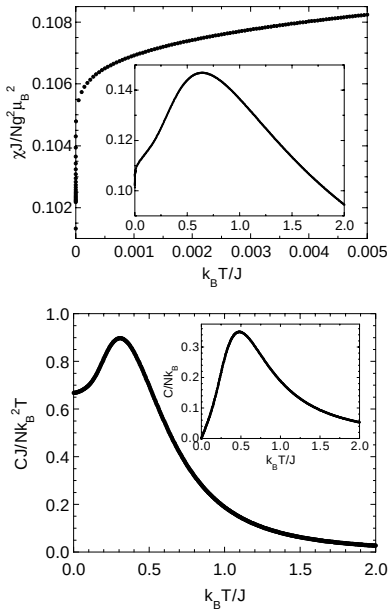


Approach

• Carry out numerical calculations of $\chi(T)$ for the S = 1/2 uniform and alternating-exchange Heisenberg chain using Bethe ansatz calculations, quantum Monte Carlo (QMC) simulations and transfer-matrix density-matrix renormalization group (TMRG) calculations. Bethe ansatz calculations of the specific heat are also performed for the uniform chain
• Obtain high-precision fits to the numerical data
• Model the experimental data with the theory

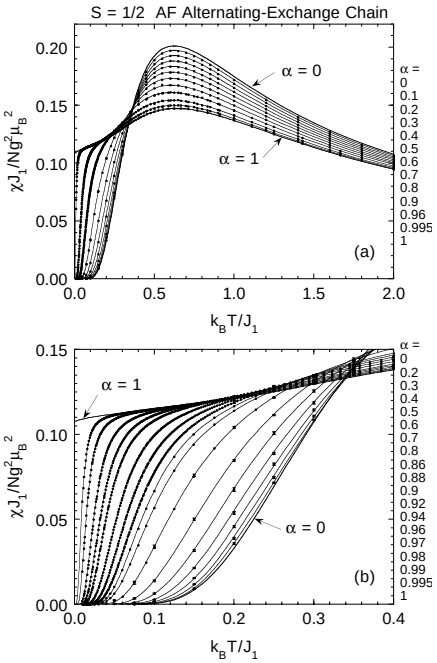
Theory

Bethe ansatz $\chi(T)$ and specific heat C(T) data for the AF S = 1/2 uniform Heisenberg chain



• The very low-temperature data are in excellent agreement with Lukyanov's 1998 exact field theory predictions

Numerical QMC and TMRG data for AF alternating-exchange chains with various values of $\alpha = J_2/J_1$



• The above set of solid curves is a single high-accuracy two-dimensional fit to the data with $0 \le \alpha \le 1$ and $0.01 \le k_BT/J_1 \le 5$. This function has been sought by experimentalists for several decades

The $\chi(T)$ function is recast below in terms of the average $J = (J_1 + J_2)/2$ and dimerization parameter $\delta = (J_1 - J_2)/2J$ instead of J_1 and $\alpha = J_2/J_1$. This form is more transparent for modeling $\chi(T)$ data for compounds containing chains with weak alternation and/or that show spin-dimerization transitions